On the relations between reversibility and lumpability

Andrea Marin, Sabina Rossi

Università Ca' Foscari Venezia
DAIS

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Section 1

Reversibility on CTMC

Background on Continuous time Markov chains

- We consider Markov chains in continuous time (CTMCs) $X(t)$
- State space S with $i, j \in S$
- $\mathbf{Q}$ is the infinitesimal generator, and
  - q_{ij} transition rate from state i to j, $i \neq j$
  - $q_{ii} = -\sum_{j \neq i} q_{ij}$
  - $q_i = -q_{ii}$ total flow out of state i
- The steady-state distribution π is the unique vector of positive numbers π_i with $i \in S$, summing to unit and satisfying the system of global balance equations (GBEs)

$$\pi \mathbf{Q} = \mathbf{0}$$

Background on time-reversible Markov chains

- Let $X(t)$ be a stationary Markov chain
- $X(\tau - t)$ is still a stationary Markov chain
- If $X(t)$ and $X(\tau - t)$ are probabilistically indistinguishable for any τ and t in the time domain, then we say that $X(t)$ is reversible
- We denote by $X^R(t)$ is the CTMC associated with $X(t)$ at reversed time, $\mathbf{Q}^R$ is its infinitesimal generator

How to derive $X^R(t)$ for stationary Markov processes?

- Assume ergodicity and let π_i be the stationary probability of state i
- Let q_{ij} for $i \neq j$ be the transition rate in a CTMC from state i to state j
- In $X^R(t)$ there exists a transition from j to i whose rate is:

$$q_{ji}^R = \frac{\pi_i}{\pi_j} q_{ij}$$

Detailed balance equations for reversibility

- $X(t)$ is reversible iff the following system of detailed balance equations is satisfied:

$$\pi_i \, q_{ij} = \pi_j \, q_{ji}$$

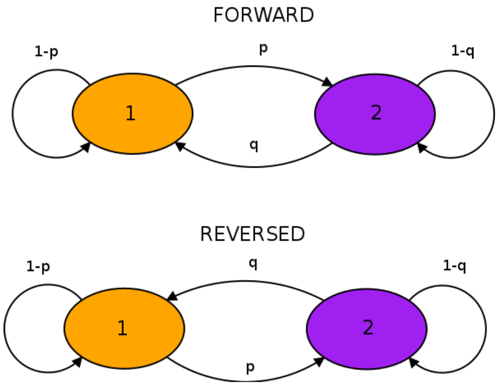
for all $i, j \in S$ with $i \neq j$.

Kolmogorov's criterion for reversibility

- $X(t)$ is reversible iff for every finite sequence of states $i_1, i_2, \ldots i_n \in S$,

$$q_{i_1 i_2} q_{i_2 i_3} \cdots q_{i_{n-1} i_n} q_{i_n i_1} = q_{i_1 i_n} q_{i_n i_{n-1}} \cdots q_{i_3 i_2} q_{i_2 i_1}$$

Example: reversibility



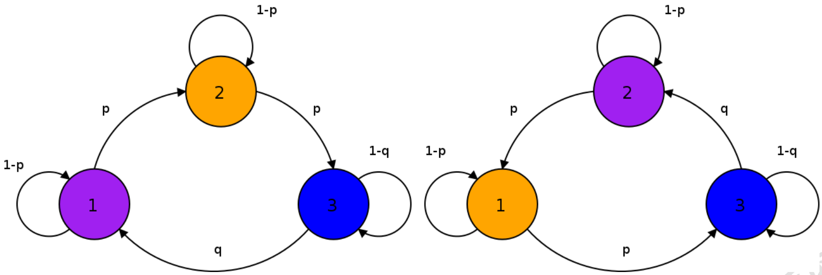
Section 2

ρ-Reversibility on CTMC

Dynamic reversibility

- Let ξ be an involution on the state space of a CTMC
  - ξ is bijective
  - $\xi(\xi(i)) = i$
- A CTMC is dynamically reversible if $X(t)$ and $X^R(t)$ are identical modulo the renaming of states ξ
- It has been used to study the properties of crystal growth and other physical systems

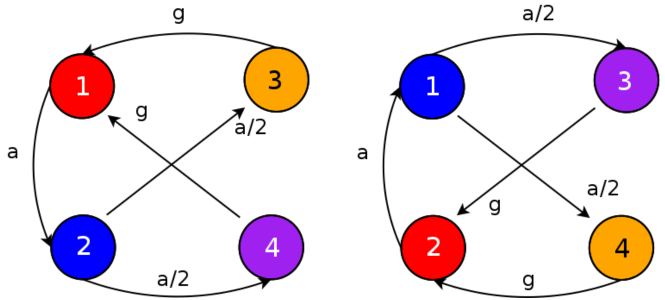
Example: dynamic reversibility



ρ-reversibility

- Let ρ be a general bijection between the state space and itself
- We say that $X(t)$ is ρ-reversible if $X(t)$ and $X^R(t)$ are stochastically indistinguishable modulo the renaming ρ
- Notice that ξ and ρ may not be unique!

Example of ρ-reversibility



ρ-Detailed balance equations for ρ-reversibility

- Let $q_i = \sum_{j \neq i} q_{ij}$
- $X(t)$ is ρ-reversible iff
  - $q_i = q_{\rho(i)}$ for all $i \in S$, and
  - the following system of detailed balance equations is satisfied:

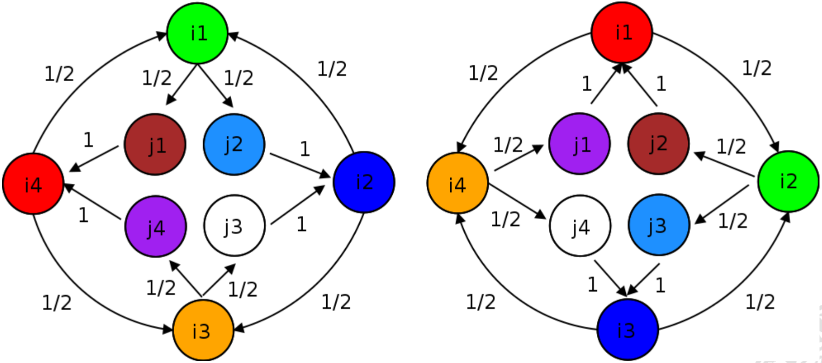
$$\pi_i \, q_{ij} = \pi_j \, q_{\rho(j)\rho(i)}$$

ρ-Kolmogorov's criterion for ρ-reversibility

- $X(t)$ is ρ-eversible iff
  - $q_i = q_{\rho(i)}$ for all $i \in S$, and
  - for every finite sequence of states $i_1, i_2, \ldots i_n \in S$

$$q_{i_1 i_2} \cdots q_{i_{n-1} i_n} q_{i_n i_1} = q_{\rho(i_1)\rho(i_n)} q_{\rho(i_n)\rho(i_{n-1})} \cdots q_{\rho(i_2)\rho(i_1)}$$

ρ-reversibility example



Permutation consisting of two cycles: $(i_1, i_2, i_3, i_4)(j_1, j_2, j_3, j_4)$

Verify ρ-reversibility with a guessed π: ρ-detailed balance equations

- Assume you have a collection π_i of positive real numbers summing to unity associated with each state i
- If for all the states it holds that:
  - $q_i = q_{\rho(i)}$ and
  - $\pi_i q_{ij} = \pi_j q_{\rho(j)\rho(i)}$

  then
  - The CTMC is ρ-reversible
  - π_i is the stationary probability of state i

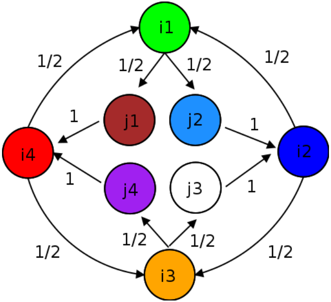
Structurally verify ρ-reversibility: ρ-Kolmogorov's criteria

- A chain is ρ-reversible if and only if for every finite sequence of state $i_1, i_2, \dots, i_n$ it holds:

$$q_{i_1 i_2} q_{i_2 i_3} \cdots q_{i_{n-1} i_n} q_{i_n i_1} = q_{\rho(i_1)\rho(i_n)} q_{\rho(i_n)\rho(i_{n-1})} \cdots q_{\rho(i_2)\rho(i_1)}$$

- For every cycle the product of its transition probabilities and those of the renamed inverse cycle must be the same
- No need to derive the reversed process
- Only minimal cycles must be checked

Example



- $i_1 \to j_2 \to i_2 \to i_1$: $\frac{1}{2}\,1\,\frac{1}{2} = \frac{1}{4}$
- $i_2 \to i_3 \to j_3 \to i_2$: $\frac{1}{2}\,\frac{1}{2}\,1 = \frac{1}{4}$

Computing the steady-state probability

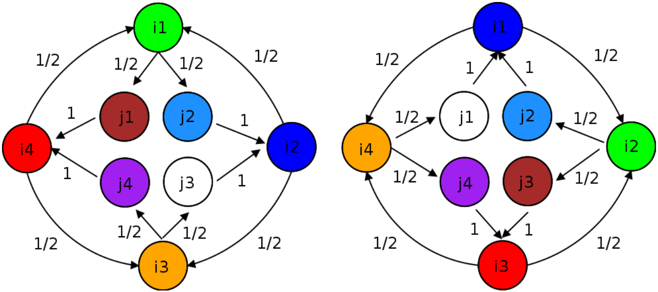
- Fix a reference state i_0
- You want to determine π_i
- Find a path from i to i_0 and determine the inverse from $\rho(i_0)$ to $\rho(i)$:

$$i = i_n \to i_{n-1} \to i_{n-2} \to i_{n-3} \to \cdots \to i_0$$

- Compute π_i as:

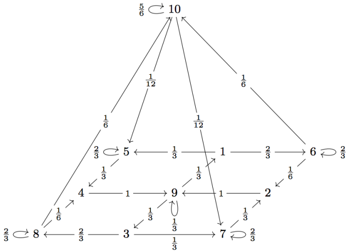
$$\pi_i = \pi_{i_0} \prod_{k=1}^{n} \frac{q_{\rho(i_{k-1})\rho(i_k)}}{q_{i_k i_{k-1}}}$$

Example



Involution: $(i_1, i_2)(i_3, i_4)(j_1, j_3)(j_2)(j_4)$

Counter-example



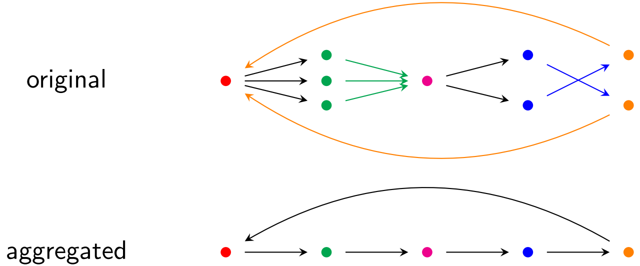
- $\rho : (1, 2, 3, 4)(5, 6, 7, 8)(9)(10)$
- No possible involution
- The class of ρ-reversible chains strictly includes dynamically reversible chains

Section 3

Lumpability on CTMC

Lumpability

The notion of *lumpability* is used for generating an aggregated Markov process that is smaller than the original one



- It can be formalized in terms of equivalence relations

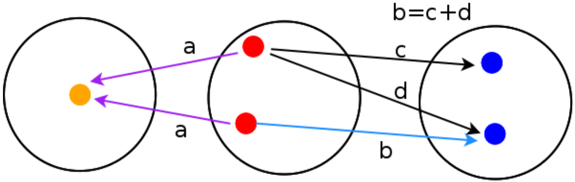
Strong lumpability

Definition

$X(t)$ is strongly lumpable w.r.t. equivalence relation $\sim$ on S if for any $[k] \neq [l]$ and $i, j \in [l]$,

$$q_{i[k]} = q_{j[k]}$$

where $q_{i[k]} = \sum_{j \in [k]} q_{ij}$.



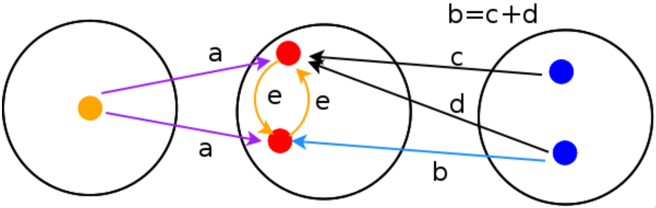
Exact lumpability

Definition

$X(t)$ is exactly lumpable with respect to $\sim$ if for any $[k], [l]$ and $i, j \in [l]$,

$$q[k]i = q[k]j$$

where $q_{[k]i} = \sum_{j \in [k]} q_{ji}$.



Strict lumpability

Definition

$X(t)$ is strictly lumpable w.r.t. equivalence relation $\sim$ on S if it is both strong and exact w.r.t. $\sim$

Notes:

- If $\sim$ is a strong lumping then $\widetilde{X}(t)$ is a CTMC (and vice versa)
- If $\sim$ is an exact lumping then all the states in the same equivalence class are equiprobable in steady-state

Section 4

Relations between lumpability and reversibility

Exact lumpability and reversed processes

Theorem

If $X(t)$ is exactly lumpable w.r.t. $\sim$ then $\sim$ is a strong lumping for $X^R(t)$

Proof sketch:

- Exact lumpability checks incoming rates to the states which become outgoing rates when reversing the process
- States belonging to the same class have the same stationary distributions

Strict lumpability and reversed processes

Theorem

$X(t)$ is strictly lumpable w.r.t. $\sim$ if and only if $\sim$ is a strict lumping also for $X^R(t)$

Theorem

If $X(t)$ is strictly lumpable w.r.t. $\sim$ then the processes $(\widetilde{X})^R(t)$ and $\widetilde{X^R}(t)$ are stochastically identical.

Section 5

$\lambda\rho$-Reversibility

λ-reversibility and ρ-reversibility

Definition

$X(t)$ λ-reversible w.r.t. to strict lumping $\sim$ such that $\widetilde{X}(t)$, $\widetilde{X^R}(t)$ are stochastically identical

Definition

$X(t)$ is ρ-reversible w.r.t. a renaming ρ on S on S such that $X(t)$ and $\rho(X^R)(t)$ are stochastically identical

$\lambda\rho$-reversibility and detailed balance equations

Definition

$X(t)$ is $\lambda\rho$-reversible w.r.t. an equivalence relation $\sim$ and a renaming ρ on $S/\sim$ if $\widetilde{X}(t)$ and $\rho(\widetilde{X^R})(r)$ are stochastically identical

Theorem

$X(t)$ is $\lambda\rho$-reversible w.r.t. $\sim$ and ρ if and only if there exists a collection of positive number $\pi_{[i]}$ $[i] \in S/\sim$ such that for all states i it holds that:

- $|[j]|\pi_i q_{i[j]} = |[i]|\pi_j q_{j'\rho[i]}, \; j' \in \rho[j]$
- $q_{[i]} = q_{\rho[i]}$

In this case π is also the statioanry distribution of $X(t)$.

Deciding $\lambda\rho$-reversibility by Kolmogorov's criterion

Theorem

$X(t)$ is $\lambda\rho$-reversible w.r.t. $\sim$ and ρ on $S/\sim$ if and only if:

- $q_{[i]} = q_{\rho[i]}$
- *For each finite cycle of states $i_1, i_2, \ldots, i_n, i_1$ we have:*

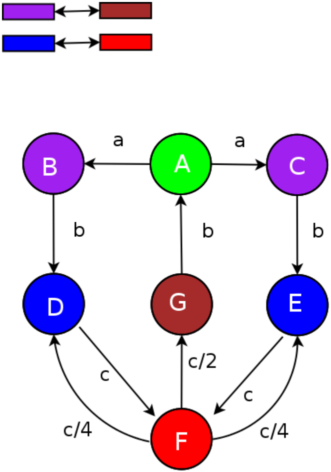
$$q_{i_1,[i_2]} q_{i_2,[i_3]} \cdots q_{i_n,[i_1]} = q_{i'_1,\rho[i_n]}, q_{i'_n,\rho[i_{n-1}} q_{i'_2,\rho[i_1]}$$

Expression of stationary distribution

How do we compute the stationary distribution?

- Fix a reference state i
- Consider a state j and choose an arbitrary path Ψ from j to i
- Let Ψ' be the path from the renaming of i to the renaming of j
- $\pi_{[j]}/\pi_{[i]}$ is equal to the product of the rates in Ψ' over the product of the rates in Ψ

Example



- Reference state A, compute π_F
- Path from F to A: $F \xrightarrow{c/2} G \xrightarrow{b} A$
- Path from A to D/E: $A \xrightarrow{2a} B \xrightarrow{b} D$

$$\pi_F = \frac{2ab}{bc/2} = \frac{4a}{c}$$

Section 6

Reversible computing

Reversible Computing

- Reversible computing is a paradigm of computation that extends the standard forward-only programming to reversible programming
  - Reversible executions may restore a past state by undoing, one by one, all the previously performed operations

Reversible Computing: Implementation

- Reversible computing can be implemented in essentially two ways:
  - by recording a set of checkpoints that store the state of the processor at some epochs of the computation
  - by implementing fully reversible programs where each step of the computation may be inverted

Contribution

- We define quantitative stochastic models for concurrent and cooperating reversible computations that are
  - stochastic automata with underlying CTMCs
- We introduce the class of *reversible stochastic automata* that
  - is closed under synchronization
  - have a product-form solution, i.e., the equilibrium distribution of the composition of reversible automata can be derived as the product of the equilibrium distributions of each automaton in isolation

Stochastic Automata

- We consider concurrent stochastic automata with underlying continuous time Markov chains
- Complex automaton can be constructed from simpler components by a *synchronization operator*
  - We distinguish between *active* and *passive* action types
  - Only active/passive synchronisations are permitted, like, e.g., in SAN, PEPA, ...

Stochastic Automata (SA)

Definition

A stochastic automaton P is a tuple

$$(\mathcal{S}_P, \mathcal{A}_P, \mathcal{P}_P, \to_P)$$

- $\mathcal{S}_P$: *state space* of P
- $\mathcal{A}_P$: set of *active* types $\mathcal{P}_P$: set of *passive* types
- τ: *unknown* type
- $\to_P$ transition relation where
  - $s_1 \xrightarrow{(a,r)}_P s_2$: $r \in \mathbb{R}^+$ is a *rate* and $a \in \mathcal{A}_P \cup \{\tau\}$
  - $s_1 \xrightarrow{(a,p)}_P s_2$: $p \in (0,1]$ is a *probability* and $a \in \mathcal{P}_P$

SA synchronisation

$$\frac{s_{p_1} \xrightarrow{(a,r)}_P s_{p_2} \quad s_{q_1} \xrightarrow{(a,p)}_Q s_{q_2}}{(s_{p_1}, s_{q_1}) \xrightarrow{(a,pr)}_{P\otimes Q} (s_{p_2}, s_{q_2})}$$

$$a \in \mathcal{A}_P = \mathcal{P}_Q$$

$$\frac{s_{p_1} \xrightarrow{(\tau,r)}_P s_{p_2}}{(s_{p_1}, s_{q_1}) \xrightarrow{(\tau,r)}_{P\otimes Q} (s_{p_2}, s_{q_1})}$$

CTMC underlying a closed SA

- P is *closed* if $\mathcal{P}_P = \emptyset$

Definition

The CTMC $X_P(t)$ underlying a closed automaton P has state space $\mathcal{S}_P$ and infinitesimal generator matrix $\mathbf{Q}$ such that for all $s_1 \neq s_2 \in \mathcal{S}_P$,

$$q(s_1, s_2) = \sum_{s_1 \xrightarrow{(a,r)}_P s_2} r$$

- π_P: equilibrium distribution of the CTMC underlying P

Reversible Stochastic Automata

- We assume that for each forward action type a there is a corresponding backward type $\overleftarrow{a}$ with $\overleftarrow{\tau} = \tau$
- Formally $\overleftarrow{\cdot}$ is a bijection (renaming)
- We say that $\overleftarrow{\cdot}$ respects the active/passive types:
  - $\overleftarrow{\tau} = \tau$
  - $a \in \mathcal{A}_P \Leftrightarrow \overleftarrow{a} \in \mathcal{A}_P$
  - $a \in \mathcal{P}_P \Leftrightarrow \overleftarrow{a} \in \mathcal{P}_P$
- We consider a bijection $\rho : \mathcal{S}_P \to \mathcal{S}_P$

Reversible Stochastic Automata

Definition

P is reversible if

- $q(s, a) = q(\rho(s), a) \qquad \forall s \in \mathcal{S}_P$;
- for all

$$\Psi = s_1 \xrightarrow{(a_1, r_1)} s_2 \xrightarrow{(a_2, r_2)} \ldots s_n \xrightarrow{(a_n, r_n)} s_1$$

  there exists an inverse cycle

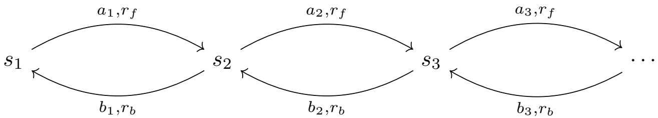
$$\overleftarrow{\Psi} = \rho(s_1) \xrightarrow{(\overleftarrow{a}_n, t_n)} \rho(s_n) \ldots \xrightarrow{(\overleftarrow{a}_2, t_2)} \rho(s_2) \xrightarrow{(\overleftarrow{a}_1, t_1)} \rho(s_1)$$

  such that:

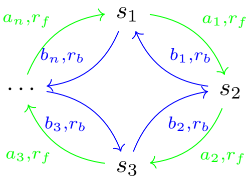
$$\prod_{i=1}^{n} r_i = \prod_{i=1}^{n} t_i$$

Examples

Infinite state model: $\rho = id$, $\overleftarrow{a}_i = b_i$, $\overleftarrow{b}_i = a_i$

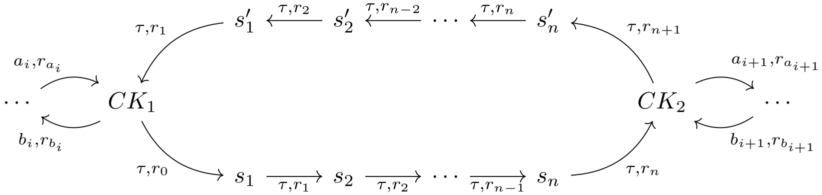


Finite state model: $\rho = id$, $\overleftarrow{a}_i = b_i$, $\overleftarrow{b}_i = a_i$, $r_f = r_b$



Example: Reversible computations with checkpoints

$$\rho(CK_i) = CK_i,\ \rho(s_i) = s_i',\ \rho(s_i') = \rho(s_i) \text{ and } \overleftarrow{a}_i = b_i,\ \overleftarrow{b}_i = a_i$$



Detailed balance equations

- We prove a necessary condition for reversibility expressed in terms of the equilibrium distribution and the transition rates

Theorem (Detailed balance equations)

If P is reversible then $\forall s, s' \in \mathcal{S}_P$, and $\forall$ action type a

$$\pi_P(s)q(s,s',a) = \pi_P(s')q(\rho(s'),\rho(s),\overleftarrow{a})$$

Equilibrium probability of the renaming of a state

- The states of an ergodic reversible automaton have the same equilibrium probability of the corresponding image under ρ

Theorem

Let P be reversible automaton. Then for all $s \in \mathcal{S}_P$,

$$\pi_P(s) = \pi_P(\rho(s))$$

Scaled automaton

- Any reversible automaton can be rescaled allowing one to close the automaton by assigning the same rate to each passive action with a certain label weighted on its probability, while maintaining the equilibrium distribution

Scaled automaton

Let a be an action type and $k \in \mathbb{R}^+$.

Definition

$S = P\{a \cdot k\}$ is defined by

- $\mathcal{S}_S = \mathcal{S}_P$
- $\mathcal{A}_S = \mathcal{A}_P$ and $\mathcal{P}_S = \mathcal{P}_P$ if $a \in \mathcal{A}_P \cup \{\tau\}$
- $\mathcal{A}_S = \mathcal{A}_P \cup \{a\}$ and $\mathcal{P}_S = \mathcal{P}_P \setminus \{a\}$ if $a \in \mathcal{P}_P$
- $\rightarrow_S \; = \; \rightarrow_P$ except for $s_1 \xrightarrow{(a,pk)}_S s_2$ if $s_1 \xrightarrow{(a,p)}_P s_2$

Reversible scaled automaton

- Let $[a]$ such that $a \in [a]$, $\overleftarrow{a} \in [a]$, $\overleftarrow{\overleftarrow{a}} \in [a]$
- $[\tau] = \{\tau\}$.

Theorem

If P is reversible, then for all action type a, then

$$P' = P\{[a] \cdot k, \} \text{ is reversible}$$

Moreover, $\pi_P(s) = \pi_{P'}(s)\ \forall s \in \mathcal{S}_P$.

Reversible scaled automaton

- The ergodicity and the equilibrium distribution of a reversible automaton does not depend on the rescaling of all the types belonging to an orbit of $\overleftarrow{\cdot}$
- If the automaton is open and we close it by rescaling, its equilibrium distribution and ergodicity does not change with the rescaling factor
- Henceforth, we will talk about equilibrium distribution and ergodicity of open automata in the sense that they are the same for any closure obtained by rescaling

Closure of reversibility under synchronization

The synchronisation of reversible automata is still ρ-reversible

Theorem

Let P be ρ-reversible and Q be σ-reversible. Then

- *$P \otimes Q$ is ξ-reversible where*

$$\xi(s_p, s_q) = (\rho(s_p), \sigma(s_q)) .$$

Product-form solution

The composition of two reversible automata has an equilibrium distribution that can be derived by the analysis of the isolated synchronizing automata

Theorem

- *Let P be ρ-reversible and Q be σ-reversible*
- *Let $\boldsymbol{\pi}_P$ and $\boldsymbol{\pi}_Q$ be the equilibrium distributions of P and Q*

If $S = P \otimes Q$ is ergodic then

$$\pi_S(s_p, s_q) = \pi_P(s_p)\pi_Q(s_q)$$

i.e., the composed automaton S exhibits a product-form solution.

Reversible scaled automaton

- Notice that this product-form solution does not require a re-parameterisation of the cooperating automata
  - the expressions of the equilibrium distributions of the isolated automata are *as if* their behaviours are stochastically independent although they are clearly not

Conclusion: Main result

Main result:

- The equilibrium distribution of any reversible stochastic automaton is insensitive to any reversible context
  - our theory allows for the definition of system components whose equilibrium performance indices are independent of their context